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SOLUTION OF A NON-LINEAR INTEGRAL EQUATION APPEARING IN THE THEORY OF AN AEROSOL

by B. Friedman, M. Shaffman,
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A Memorandum Submitted
by the
Applied Mathematics Group, New York University
to the
Applied Mathematics Panel
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April 1944

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INTRODUCTION

The present study arose in connection with a mathematical problem in the field of diffusion theory, and was undertaken by the New York University Group of the Applied Mathematics Panel at the request of Division 10 of the N.D.R.C. It was carried out by Dr. B. Friedman and Dr. M. Shiffman with the assistance of E. Isaacson.

An aerosol is a suspension of liquid particles in air, such as vapor or smoke. By mutual collisions, particles will coagulate; by gravity, particles will settle on the ground and disappear from the aerosol. The problem is to determine the number $N(R,T)$ of particles of radius R at any time T, provided that the probability of collision and that of settling are known* and that the number N of particles of radius R at the time $T = 0$ is given as a function of R.

The corresponding mathematical problem is that of solving the initial value problem of a non-linear integro-differential equation of the "convolution type". This equation sets the rate of change of the number $N(R,T)$ of particles equal to the rate of creation of these particles by coagulation of smaller particles, minus the rate at which the particles of radius R collide with other particles and minus the rate at

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* These probability functions were determined long ago by Smoluchowski who seems to have been the first to investigate the coagulation problem. The settling term was included by Dr. Goldman of Division 10 of the N.D.R.C., who derived the integral equation, the solution of which is the subject of the present memorandum.

which they settle.

In the present paper a solution of the problem is given provided the initial distribution $N(R,0)$ is homogeneous, i.e., all the particles have the same radius. The procedure is not essentially different from Smoluchowski's method and is based on a reduction to a system of ordinary differential equations.

In a subsequent memorandum a solution of the integro-differential equation for non-homogeneous initial distributions will be presented. Such an extension of the theory is desirable since in practice aerosols may not be initially homogeneous. The generalized method will likewise apply to a larger class of functional equations of diffusion.

R. Courant
Contractor's Technical Representative

SOLUTION OF A NON-LINEAR INTEGRAL EQUATION APPEARING IN THE THEORY OF AN AEROSOL

1. The Integral Equation.

The behavior of an aerosol, i. e., a suspension of spherical liquid particles in air, is of interest in many practical applications. The particles, in the course of their random motion, collide with one another and coagulate to form larger particles. In addition, some particles settle to the bottom of the air container by the action of gravity, and so disappear from the suspension. A quantitative theory of this action was developed by Dr. D. E. Goldman,* who derived a non-linear integro-differential equation on the basis of kinetic theory. This memorandum takes the integral equation as a starting point and offers a solution. A statement of Dr. Goldman's result follows:

Let $N(R,T)dR$ be the concentration of particles of radii between R and $R+dR$ at time T. It is required to find $N(R,T)$ given the initial distribution $N(R,0)$. For any fixed R, the number of particles will change with time because of the following factors:

1. Particles of size R will be destroyed by collision with particles of any other size.

2. Particles of size R will be created by the coagulation of smaller particles.

3. Particles of size R will settle under the influence of gravity.

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* In a manuscript dated 11-29-43, for Section 10.2, NDRC.

Expressing these effects mathematically, the following equation was obtained by Goldman:

$$(1) \qquad \frac{\partial N(R,T)}{\partial T} = -\frac{K_o}{2}\int_{v_o}^{\infty} \phi(X,R)N(R,T)N(X,T)dX + \frac{K_o}{4}\int_{X^3+Y^3=R^3} \phi(X,Y)N(X,T)N(Y,T)\frac{dY}{dR}\,dX^{*} - U(R)N(R,T),$$

where $\phi(X,Y)$ and $U(R)$ are the following functions:

$$\phi(X,Y) = \left[\frac{X+\alpha}{X^2} + \frac{Y+\alpha}{Y^2}\right](X+Y)$$

$$U(R) = \beta R(R+\alpha).$$

The constants α, β and K_o are defined as follows: α is connected with the mean free path of the air molecules and can be taken as

$$\alpha = .083 \text{ microns} = .083 \times 10^{-4} \text{ cm.},$$

$$\beta = 2\rho g/9\eta h = 1.27 \times 10^{6}\ \rho/h,$$

$$K_o = 4KT/3\eta = 3 \times 10^{-10} \text{ (for } T = 273^{\circ} \text{ absolute)}$$

where ρ is the density of the liquid, g is the gravitational acceleration, η the viscosity of the air, h the ratio of volume to floor area of the container, K is Boltzman's

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* In the second integral the range of X is from 0 to R and Y is determined by the equation $Y^3 = R^3 - X^3$. This equation expresses the fact that, in coagulation, the volumes add.

constant and T the absolute temperature. (The values of the constants are given in c.g.s. units.)

In equation (1), the individual terms on the right side represent, respectively, the effect of the destruction, creation and settling of the particles.

It is convenient to introduce non-dimensional variables r, x, y as follows: Let α be the unit of length, $1/\alpha^2\beta$ the unit of time, $2\alpha\beta/K_o$ the unit of concentration per unit radius, and $2\alpha^2\beta/K_o$ the unit of total concentration. Now set

$$(2)\quad \begin{cases} R = \alpha r, \; X = \alpha x, \; Y = \alpha y \\ T = t/\alpha^2\beta \\ N(R,T) = 2\alpha\beta\, n(r,t)/K_o \end{cases}$$

A simple integration of the last equation justifies our choice of the unit of total concentration.

When (2) is substituted in (1) we obtain

$$(3)\quad \frac{\partial}{\partial t} n(r,t) = -\int_{x_o}^{\infty} f(r,x)n(r,t)n(x,t)dx + \frac{1}{2}\int_{x^3+y^3=r^3} f(x,y)n(x,t)n(y,t)\frac{dy}{dr}\,dx - u(r)n(r,t),$$

where now

$$(4)\quad f(x,y) = \left[\frac{x+1}{x^2} + \frac{y+1}{y^2}\right](x+y)$$

and

$$u(r) = r(r + 1) . \tag{5}$$

The problem before us now is to solve the integral equation (3) given the initial distribution $n(r,0)$.

The equation (3) is a 'reduced' equation, which does not involve any physical constants. This shows that if two aerosols have the same reduced initial distribution $n(r,0)$, they have similar behavior.

2. Summary of the Results

In this memorandum the problem is solved under the assumption that the initial distribution in the aerosol is homogeneous, i.e., particles of only one size are present.

Let the initial distribution have a (non-dimensional) concentration n_1 of particles of a single radius r_1. By coagulation, particles of twice the mass, or of radius $\sqrt[3]{2}r_1$ are formed. By further collisions and coagulations, particles of radii $\sqrt[3]{3}r_1$, $\sqrt[3]{4}r_1$, etc. will appear. For convenience denote $\sqrt[3]{2}r_1$, $\sqrt[3]{3}r_1$, $\sqrt[3]{4}r_1$, etc., by r_2, r_3, r_4, etc. respectively.

Let $n_1(t)$, $n_2(t)$, $n_3(t)$, etc., denote the concentration of particles, at any time t, of radii r_1, r_2, r_3, etc., respectively. The particles of radius r_2 are created rapidly at the beginning, while those of radii r_3, r_4, etc., are created very slowly. For practical purposes we can therefore set $n_3(t) = n_4(t) = \ldots = 0$.

The solutions for $n_1(t)$ and $n_2(t)$ are divided into two cases depending on whether the settling or collision term is initially predominant. If the settling term predominates over the collision term, we obtain the formulas:

$$(6)\qquad n_1(t) = \frac{n_1(1 - A^2)}{e^{u_1 t} - A^2}$$

$$(7)\qquad n_2(t) = n_1(t)\cdot\frac{1}{2} A e^{-.6u_1 t} \log\left[\frac{1 + A}{1 - A}\cdot\frac{e^{\frac{u_1}{2}t} - A}{e^{\frac{u_1}{2}t} + A}\right],$$

where $A^2 = \dfrac{f_{11}n_1}{u_1 + f_{11}n_1}$, $u_1 = u(r_1)$, $f_{11} = f(r_1, r_1)$.

These formulas are accurate if A is small, i.e., if the magnitude of u_1 is greater than, or equal to, that of $f_{11}n_1$, and the accuracy increases as $\dfrac{u_1}{f_{11}n_1}$ increases.

If, on the other hand, the collision term is the predominant one, we get the following formulas:

$$(8)\qquad n_1(t) = n_1 e e^{-(1 + w)^2} e^{- u_1 t}$$

$$(9)\qquad n_2(t) = n_1 e w e e^{-(1 + w)^2} e^{-u_2 t},$$

where $u_2 = u(r_2)$, and where w is related to t by the equation

$$(10)\qquad \frac{u_1}{n_1 e f_{11}} \int_0^w e(1 + w)^2 dw = 1 - e^{-\frac{u_1}{2} t} .$$

The integral is tabulated in Jahnke-Emde (1943 Ed.) p.32,

since it can be written as $\int_1^{w+1} e^{s^2} ds$. (The use of the tables accounts for the seemingly awkward form of equations (8), (9), (10) involving e.) These formulas are quite accurate if u_1 is of a smaller order of magnitude than $n_1 f_{11}$, and the accuracy increases as $u_1/f_{11}n_1$ decreases.

As functions of time, the foregoing formulas are especially accurate when t is small. In section 3, a comparison of the formulas for a special case with a numerical solution illustrates these points.

3. Solution for a Special Case.

A solution has been carried out in one test case. This special problem was selected as a case on the borderline between the two possibilities discussed on p. 4. Thus, in any other specific instance, the results will be at least as accurate as those under consideration here, since the accuracy is increased in either the first or the second case according as the ratio of the settling term to the collision term increases or decreases.

The example selected is $r_1 = 10, n_1 = 100$. Here $u_1 = 110$, $f_{11}n_1 = 440$ so that the collision term is slightly predominant over the settling term.

This case would correspond to the following physical situation. Suppose the density ρ of the liquid is 1 gm/cm^3 and the height h is 100 cm. The scaling factors, using the units on p. 3, are then

$\alpha = .083$ microns

$1/\alpha^2\beta = 1.2 \times 10^6$ sec.

$2\alpha\beta/K_o = 7 \times 10^8$ particles/cm^3

$2\alpha^2\beta/K_o = 5.8 \times 10^3$ particles/cm^3

The initial conditions $r_1 = 10$, $n_1 = 100$ mean an initial concentration of 5.8×10^5 particles/cm^3, all of radius .83 micron. The time scale is such that an interval of 10^{-3} in t corresponds to 20 minutes.

The equations (6) through (10) become

$$(6)' \qquad n_1(t) = 20/(e^{110t} - .8),$$

$$(7)' \qquad n_2(t) = n_1(t)\, \frac{.447}{e^{66t}} \log \left[\frac{1.894}{.106} \cdot \frac{e^{55t} - .894}{e^{55t} + .894} \right],$$

$$(8)' \qquad n_1(t) = 271.8\, e^{-(1 + w)^2} e^{-110t},$$

$$(9)' \qquad n_2(t) = 271.8\, we^{-(1 + w)^2} e^{-171t},$$

$$(10)' \qquad .0919 \int_0^w e^{(1 + w)^2} dw = 1 - e^{-55t}.$$

We also obtained a solution for this test case by numerical integration of the differential equations (12), to be derived in section 4 from the integral equation (3), neglecting terms of subscript ≥ 4. Figure 1 expresses the numerical solution in graphical form. Figure 2 gives a pictorial comparison of the numerical solution for $n_1(t)$ with the

solutions for n_1 in (6)', (8)'. Figure 3 compares the numerical solution with those obtained for n_2 in (7)', (9)'. Again we repeat, the accuracy is very good when t is small.

4. Mathematical Treatment.

In solving the integral equation (3) we assume, as was stated in section 2, that the initial distribution is homogeneous. It will be shown that (3) reduces to an infinite set of differential equations, of which only the first two need be retained, the remaining ones being negligible. (See section 2.)

Assume a homogeneous initial distribution $n(r,0)$, i.e., all the particles have the same radius r_1. This can be indicated mathematically by setting

$$n(r,0) = n_1 \delta(r-r_1)$$

where $\delta(r)$ is the δ-function and n_1 is the initial concentration.

At any time t the distribution will no longer be homogeneous, but will consist of particles of radius $r_1, r_2, \ldots, r_k, \ldots$. Denoting the concentration of particles of radius r_k by $n_k(t)$, the distribution $n(r,t)$ can then be written as

$$(11)\quad n(r,t) = n_1(t)\delta(r-r_1) + n_2(t)\delta(r-r_2) + \ldots + n_k(t)\delta(r-r_k) + \ldots .$$

By substituting this in the integral equation the following

system of differential equations is obtained:

$$(12)\quad \begin{cases} \dfrac{dn_1(t)}{dt} = -n_1(t)\left[u_1 + \sum_{j=1}^{\infty} f_{1j}n_j(t)\right] \\ \dfrac{dn_2(t)}{dt} = -n_2(t)\left[u_2 + \sum_{j=1}^{\infty} f_{2j}n_j(t)\right] + \frac{1}{2}f_{11}n_1(t)n_1(t) \\ \dfrac{dn_3(t)}{dt} = -n_3(t)\left[u_3 + \sum_{j=1}^{\infty} f_{3j}n_j(t)\right] + \frac{2}{2}f_{12}n_1(t)n_2(t) \\ \vdots \qquad\qquad \vdots \qquad\qquad \vdots \\ \dfrac{dn_k(t)}{dt} = -n_k(t)\left[u_k + \sum_{j=1}^{\infty} f_{kj}n_j(t)\right] + \frac{1}{2}\sum_{j=1}^{j=k-1} f_{j,k-j}n_j(t)n_{k-j}(t) \\ \vdots \qquad\qquad \vdots \qquad\qquad \vdots \end{cases}$$

where $u_k = u(r_k)$

and $f_{ij} = f(r_i, r_j)$

and the initial conditions are

$$n_1(0) = n_1, n_2(0) = n_3(0) = \ldots = n_k(0) = 0.$$

A closer analysis of the physical mechanism reveals that

particles of radius r_2 will be immediately and rapidly created by the coagulation of the original particles, but that particles of radius r_3 and larger are created very slowly. As a first approximation, the number of these particles can be neglected; that is, assume

$$n(r,t) = n_1(t)\ \delta(r-r_1) + n_2(t)\ \delta(r-r_2). \tag{13}$$

Then (12) reduces to

$$\begin{cases} \dfrac{dn_1(t)}{dt} = -n_1(t)\,[u_1 + f_{11}n_1(t) + f_{12}n_2(t)\,] \\ \dfrac{dn_2(t)}{dt} = -n_2(t)\,[u_2 + f_{21}n_1(t) + f_{22}n_2(t)] + \frac{1}{2}f_{11}[n_1(t)]^2 \end{cases} \tag{14}$$

with initial conditions $n_1(0) = n_1, n_2(0) = 0$.

Before we solve this system, it is well to note the following relations between the coefficients $u_1, u_2, f_{11}, f_{12}, f_{22}$. Remembering that $r_2 = \sqrt[3]{2}r_1 = 1.26r_1$, the following table can be prepared:

r_1	$\frac{f_{22}}{f_{11}}$	$\frac{f_{12}}{f_{11}}$	$\frac{u_2}{u_1}$
1	.90	.97	1.42
2	.93	.98	1.48
4	.96	1.00	1.52
6	.97	1.00	1.54
8	.98	1.00	1.55
10	.98	1.01	1.56
15	.99	1.01	1.57
∞	1.00	1.01	1.59

Thus, for all but the extremely minute particles, the coefficients f_{12}, f_{22} can be safely replaced by f_{11}, while u_2 is approximately $1.5u_1$.

Case 1. The Settling Term Predominates.

In the first equation (14) we can neglect $f_{12}n_2(t)$ because $n_2(t)$ is small compared with $n_1(t)$ in the beginning and as t increases it is still small compared with u_1. This leads to a simple differential equation for $n_1(t)$ alone, the solution of which is equation (6). (See p. 5)

Similarly, in the second of equations (14) the term $f_{22}n_2(t)$ can be neglected, leading to the differential equation

$$(15)\quad \frac{dn_2(t)}{dt} + n_2(t)\,[u_2 + f_{21}n_1(t)\,] = \tfrac{1}{2}f_{11}[n_1(t)]^2$$

where formula (6) is to be substituted for $n_1(t)$. This is a linear differential equation for $n_2(t)$, the solution of which is

$$(16)\quad n_2(t) = e^{-\int[u_2+f_{21}n_1(t)]dt} \cdot \int \tfrac{1}{2}f_{11}[n_1(t)]^2\, e^{\int[u_2+f_{21}n_1(t)]dt}\, dt$$

The quantity $\int[u_2 + f_{21}n_1(t)]dt$ can be evaluated immediately with the result

$$e^{\int[u_2 + f_{21}n_1(t)]dt} = e^{u_2 t}\,[1 - Ae^{-u_1 t}]^{f_{21}/f_{11}}$$

Making use of the very close approximation $f_{21}/f_{11} = 1$, formula (16) becomes

$$(17)\quad n_2(t) = \frac{e^{-u_2 t}}{1 - A^2 e^{-u_1 t}} \cdot \tfrac{1}{2}f_{11} \cdot \frac{u_1^2 A^4}{f_{11}^2} \int_0^t \frac{e^{-2u_1 t}\cdot e^{u_2 t}}{1 - A^2 e^{-u_1 t}}\,dt.$$

The integral can be evaluated explicitly if the further approximation $u_2 = 1.5u_1$ is made. The substitution $Ae^{-u_1 t/2} = x$ then gives

$$\int_0^t \frac{e^{-\frac{1}{2}u_1 t}\,dt}{1 - A^2 e^{-u_1 t}} = \frac{2}{u_1 A}\int_x^A \frac{dx}{1 - x^2} = \frac{1}{u_1 A}\log\left[\frac{1+A}{1-A}\cdot\frac{1 - Ae^{-u_1 t/2}}{1 + Ae^{-u_1 t/2}}\right]$$

Inserting this in (17), one finally obtains equation (7), (see page 5) where the approximation $u_2 = 1.5u_1$ has been used for the term $e^{-u_2 t}$ outside the integration sign.

Case 2. The Collision Term Predominates.

In this case the preceding equations might hold at the beginning, but would be considerably in error for large t. It is now not justifiable to neglect $f_{21}n_2(t)$ compared with $u_1 + f_{11}n_1(t)$.

From the table given previously, it is seen that f_{ij} changes slightly when i and j range from 1 to 2. Assume that f_{ij} is constant and represent it by f_1.

The equations (14) are now

$$(18)\begin{cases}\dfrac{dn_1(t)}{dt} = -n_1(t)[u_1 + f_1 n_1(t) + f_1 n_2(t)] \\ \dfrac{dn_2(t)}{dt} = -n_2(t)[u_2 + f_1 n_1(t) + f_1 n_2(t)] + \frac{1}{2}f_1[n_1(t)]^2\end{cases}$$

Let

$$(19)\quad n_2(t) = we^{(u_1 - u_2)t}n_1(t).$$

After some simplifications, the equations (18) reduce to

$$(20)\begin{cases}\dfrac{dn_1(t)}{dt} = -u_1 n_1(t) - f_1[n_1(t)]^2[1 + we^{(u_1 - u_2)t}] \\ \dfrac{dw}{dt} = \frac{1}{2}f_1 n_1(t)\, e^{-(u_1 - u_2)t}.\end{cases}$$

If the first equation is divided by the second, the result is

$$(21)\quad \frac{dn_1(t)}{dw} = -\frac{2u_1}{f_1} e^{(u_1 - u_2)t} + 2n_1(t)[e^{(u_1 - u_2)t} + we^{2(u_1-u_2)t}].$$

Introduce the new variable

$$z = e^{(u_1 - u_2)t}.$$

Then equation (21) and the second of equations (20) become

$$(22)\quad \begin{cases} \dfrac{dn_1(t)}{dw} = -\dfrac{2u_1}{f_1} z + 2n_1(t)\,[z + wz^2] \\ \dfrac{dw}{dz} = -\dfrac{f_1 n_1(t)}{2(u_1 - u_2)z^2}. \end{cases}$$

If the second equation of (22) is solved for $n_1(t)$, the result differentiated with respect to w and then substituted in the first equation, the following equation for z as a function of w is obtained:

$$(23)\quad 2z - \frac{z^2 z''}{(z')^2} = -\frac{u_1}{u_1 - u_2} z - \frac{2z^3}{z'}(1 + wz).$$

Primes denote differentiation with respect to w. The initial conditions are $z(0) = 1, z'(0) = -\dfrac{u_1}{f_1 n_1(0)} (= -k)$.

The approximation $u_2 = 1.5u_1$ simplifies (23) to

$$(24)\quad z'' = 2z'\, z(1 + wz).$$

Set $z = 1 - ky$ where $y(0) = 0$ and $y'(0) = 1$.

Equation (24) in terms of y becomes

$$ky'' = 2ky' (1 - ky) [1 + w(1 - ky)].$$

If k is small so that it may be neglected compared to 1, this equation reduces to

$$y'' = 2y' (1 + w) .$$

Its solution is

$$y = \frac{1}{e} \int_o^w e(1 + w)^2 dw$$

so that

$$z = 1 - \frac{k}{e} \int_o^w e(1 + w)^2 dw . \tag{25}$$

From the second equation of (22), $n_1(t)$ can be found to be

$$n_1(t) = n_{1e} e^{-(1 + w)^2} e^{-u_1 t} . \tag{26}$$

Then from equation (19)

$$n_2(t) = n_{1e} we^{-(1 + w)^2} e^{-u_2 t} . \tag{27}$$

Finally, the relation between w and t is found from (25) by substituting $e^{-\frac{1}{2}u_1 t}$ for z:

$$1 - e^{-\frac{1}{2}u_1 t} = \frac{u_1}{ef_1 n_1} \int_o^w e (1 + w)^2 dw. \tag{28}$$

In case an expression for the number $n_3(t)$ of particles of radius r_3 is needed, it can be found by solving this

differential equation:

$$\frac{dn_3(t)}{dt} = - n_3(t) \left[u_3 + f_{31}n_1(t) + f_{32}n_2(t) \right] + f_{12}n_1(t)n_2(t),$$

where $n_1(t)$, $n_2(t)$ are obtained from either (6), (7) or (8), (9), (10). This is a linear differential equation which can be solved by standard methods. To evaluate the resulting integrals, it may be necessary to resort to a graphical or numerical procedure.

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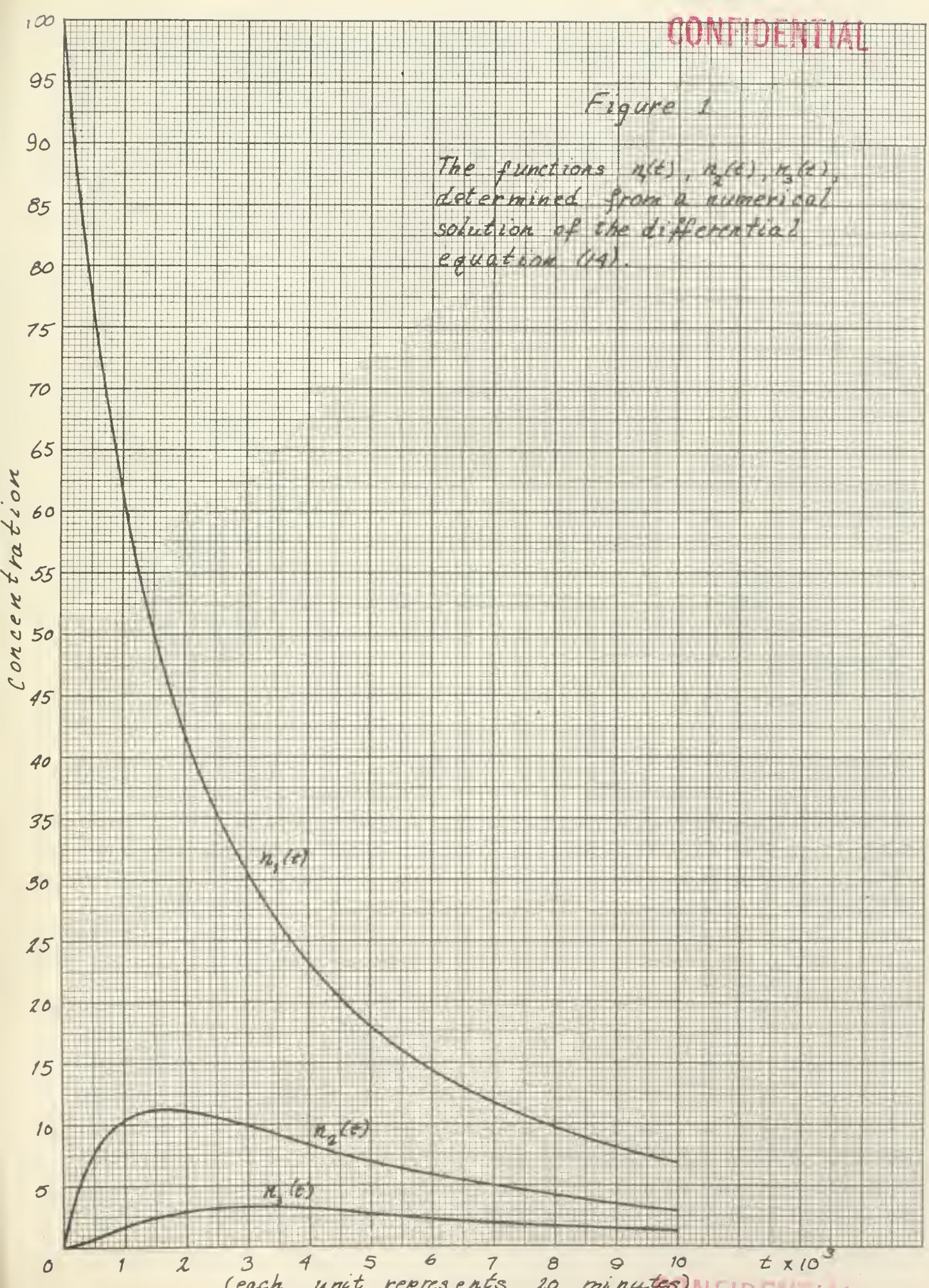
Figure 1

The functions $n_1(t)$, $n_2(t)$, $n_3(t)$, determined from a numerical solution of the differential equation (14).



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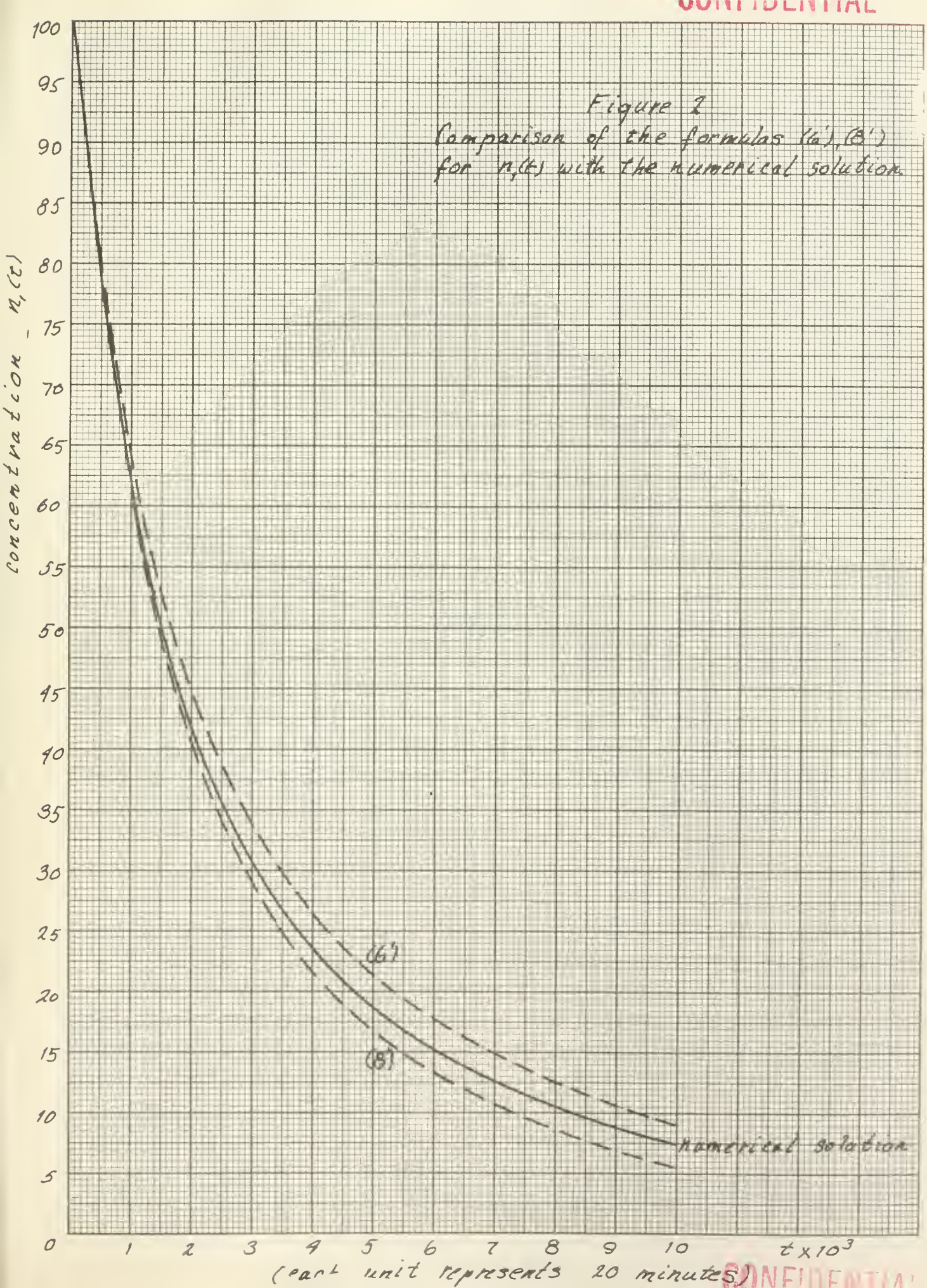

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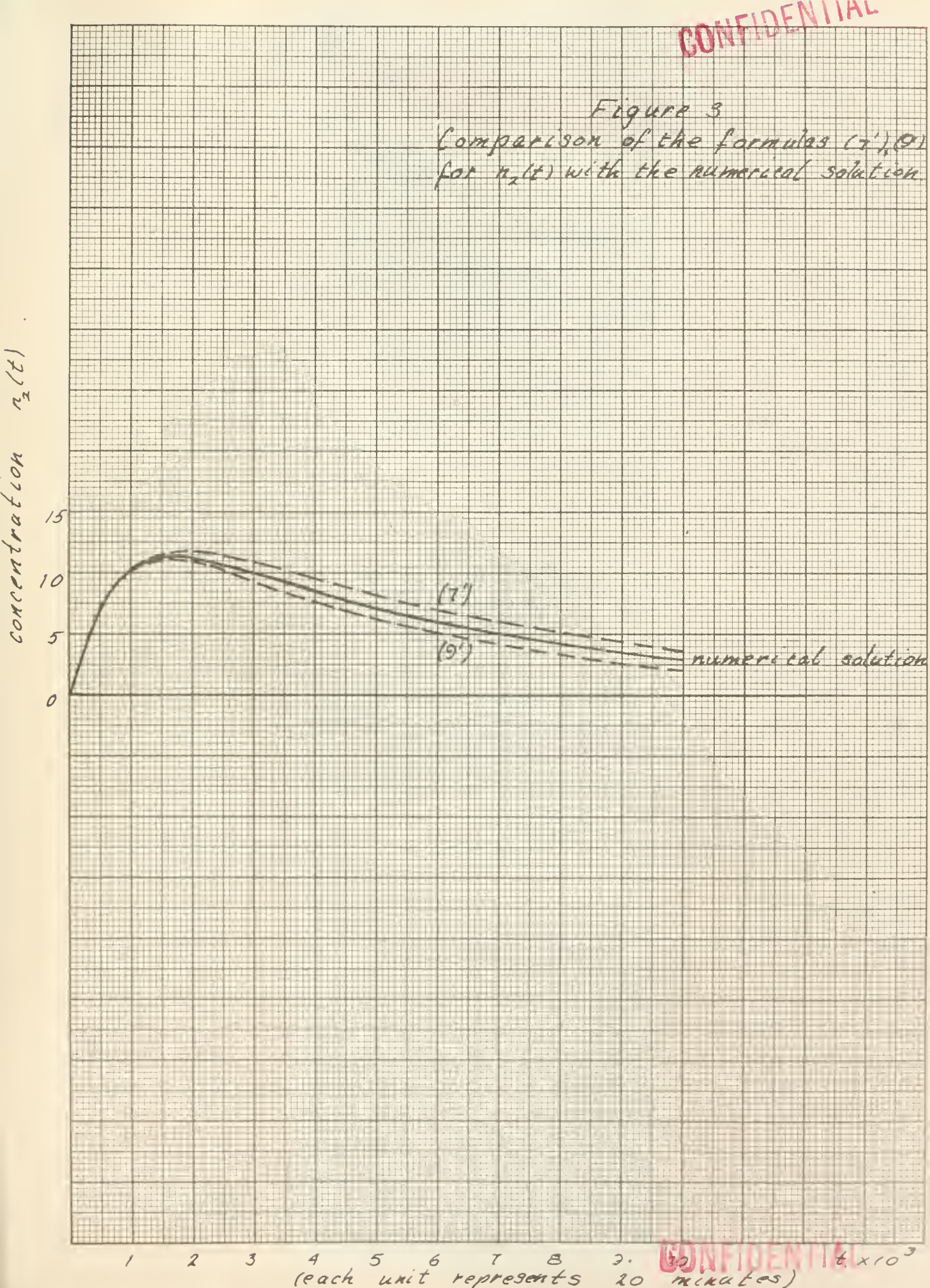
Figure 3
Comparison of the formulas (7'), (9') for $n_2(t)$ with the numerical solution



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